

2-(propan-2-yl)-1,3,6-trioxocane
15351-38-9 | DTXSID80279934

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 6.58e-02 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.23e-01

Confidence level: 5.77e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Phosmet</div> <div>Measured: 2.30e-02</div> <div>Predicted: 5.53e-07</div>	<div>Image not found</div> <div>Isopropyl octadecanoate</div> <div>Measured: 5.20e-01</div> <div>Predicted: 1.13e-05</div>	<div>Image not found</div> <div>1-Bromotetradecane</div> <div>Measured: 2.61e-02</div> <div>Predicted: 5.80e-04</div>
<div>Image not found</div> <div>2-Undecanone</div> <div>Measured: 9.89e-02</div> <div>Predicted: 6.59e-02</div>	<div>Image not found</div> <div>Octanal</div> <div>Measured: 4.00e-02</div> <div>Predicted: 9.32e-01</div>	